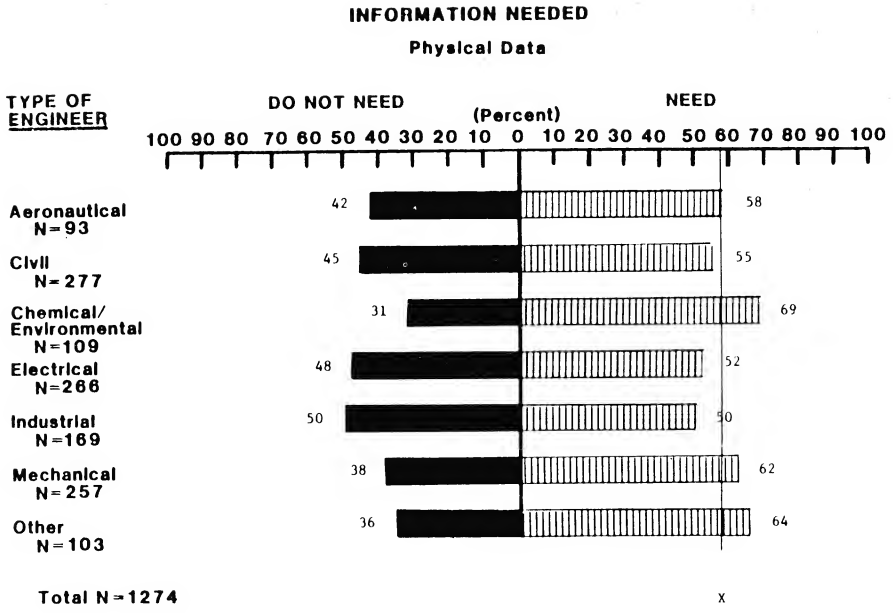


Figure 1

Figures 1 and 2 illustrate physical data requirements by type of engineer and engineering job activity.

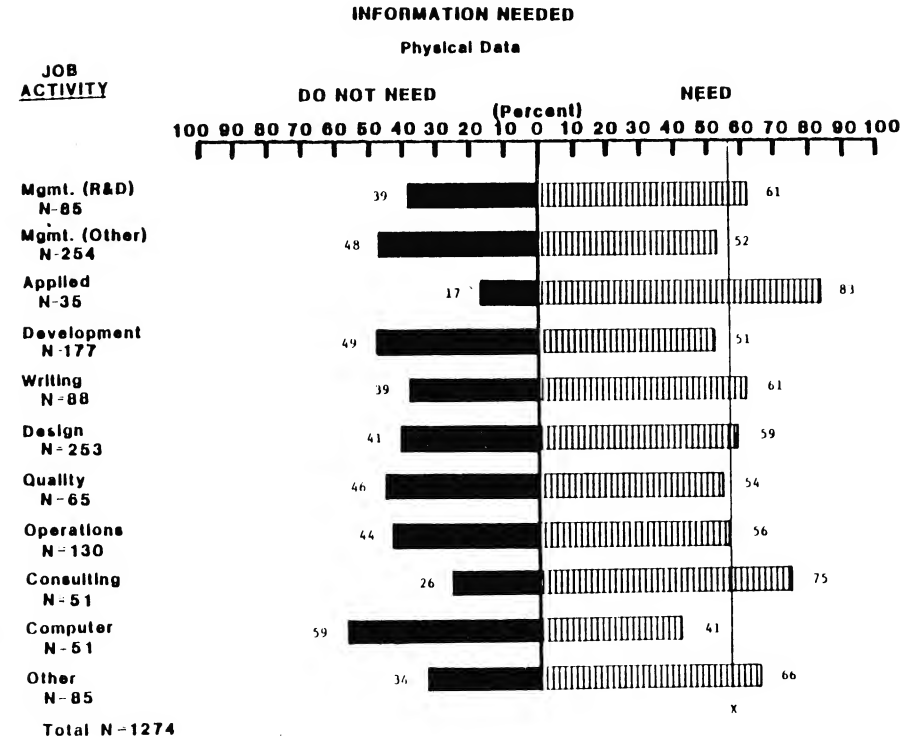


Figure 2

NEWS BRIEFS *(continued)*

The Office of Standard Reference Data organized the "Symposium on Thermodynamic Data Bases--Formulation, Reliability, and Availability" at the 181st National Meeting of the American Chemical Society in Atlanta, Georgia, March 29-April 3, 1981. Thirteen invited papers were delivered on new developments in thermodynamic data systems from all over the world.

At the accompanying technical exposition, OSRD exhibited publications and computer-readable data bases available from the Standard Reference Data Program. Highlights of the exhibit were on-line demonstrations of major computerized data bases, such as chemical thermodynamics and single crystal structural properties, and small "microdatabases" of properties of the elements, under development for possible use in educational information systems.

(continued on page 3)

NSRDS National Standard Reference Data System

Reference Data Report
Vol. 5, No. 2, 2nd Quarter 1981
S.P. Fivozinsky, Editor
C.A. Goldman, Asst. Editor

Reference Data Report is an informal communication of the National Standard Reference Data System (NSRDS) for the exchange of news and ideas about data centers, publications, meetings, and other activities related to data evaluation and dissemination. The NSRDS, which operates under the authority given in Public Law 90-396, was established to make critically evaluated data in the physical sciences available to the scientific and technical community. The NSRDS is administered and coordinated by the NBS Office of Standard Reference Data. Comments and suggestions on Reference Data Report should be addressed to:

Office of Standard Reference Data
Physics Bldg., Room A320
National Bureau of Standards
Washington, DC 20234

New Technique for Blood Serum Analysis Utilizes Evaluated Chemical Equilibrium Constants *(continued)*

Since the new method does not depend on spectrophotometric measurements, either highly turbid or non-absorbing solutions can be readily analyzed. Similar procedures should be applicable to the determination of any substrate involved in an enzyme-catalyzed reaction that releases or absorbs hydrogen ions.[1]

The ability to accurately calculate the glucose concentration in the serum was based on the availability of accurate chemical equilibrium constants provided by the NBS Electrolyte Data Center.[2] Much Data Center effort has focused on the evaluation of activities of solute and water for aqueous electrolyte systems. This thermodynamic information is of central importance when carrying out equilibrium calculations on aqueous systems and is needed to answer such commonly asked questions as: "How far does a given reaction go to completion?" and "What is the minimum energy requirement or maximum available work associated with a given process?" Recently such information has taken on enhanced value due to the widespread use of computer codes for equilibrium-modeling calculations on complex systems.[3,4]

Information produced by the Data Center is being utilized in several other interesting applications. Estimated thermodynamic data have been used in equilibrium calculations on the NH_3-CO_2-H_2S-H_2O system, which is of particular importance in coal conversion processes. Data Center staff have published evaluations leading to recommended values for activities of water in aqueous sulfuric acid and calcium chloride, systems serving as reference standards for relative vapor pressure measurements.[5,6] Evaluations have also been used to test predictions of a theoretical extension to the Debye-Hückel theory of electrolyte solutions and have served to guide experimentalists' decisions in the choice of systems to study.

Current efforts of the Data Center are focused on applications to flue gas desulfurization problems, methods for increased utilization of data in computer equilibrium codes and extensions to mixtures, and highly charged electrolyte solutions. For further information on the activities of the NBS Electrolyte Data Center, contact:

Dr. Bert R. Staples
Manager, Electrolyte Data Center
National Bureau of Standards
Washington, DC 20234

References

1. A. Mosca et al., Improved Apparatus for the Differential Measurement of pH: Applications to the Measurement of Glucose, Anal. Biochem. 112, 287 (1981).

2. R. N. Goldberg, Thermodynamics of Hexokinase Catalyzed Reactions, Biophys. Chem. 4, 215 (1976).

3. J. F. Zemaitis, Jr., Predicting Vapor-Liquid-Solid Equilibria in Multicomponent Aqueous Solutions of Electrolytes, in Thermodynamics of Aqueous Systems with Industrial Applications, (S.A Newman, editor), American Chemical Society, Washington, DC (1980).

4. T. J. Woolery, Calculation of Chemical Equilibrium Between Aqueous Solution and Minerals: the EQ3/6 Software Package, UCRL-52658, Lawrence Livermore Laboratory, Livermore, CA (1979).

5. B. R. Staples and R. L. Nuttall, The Activity and Osmotic Coefficients of Aqueous Calcium Chloride at 298.15K, J. Phys. Chem. Ref. Data 6, 385 (1977).

6. B. R. Staples, The Activity and Osmotic Coefficients of Aqueous Sulfuric Acid at 298.15K, J. Phys. Chem. Ref. Data, in press. □

NEWS BRIEFS *(continued)*

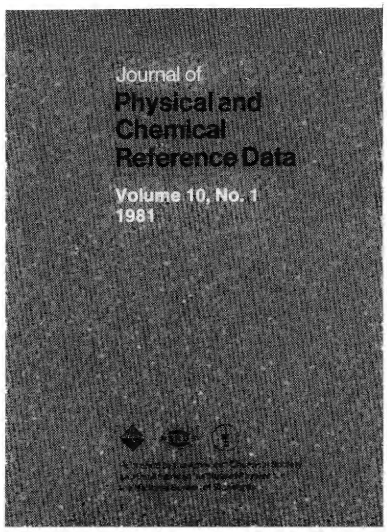
The Office of Standard Reference Data recently held a Workshop on Automation in Data Centers, May 4-5, 1981, at NBS in Gaithersburg. The workshop concerned itself with how to increase the use of computers in all aspects of data center activity, including the identification of pertinent literature, the compilation and maintenance of bibliographic and numerical data files, and the dissemination of data. The role of computers in the data evaluation process was also described.

The workshop was designed to expose data centers to presently successful use of computers by other data centers and to generate a sharing of common problems and solutions. Descriptions of on-line data distribution systems and creative uses of computer graphics and modeling were presented. About 70 persons, mostly from OSRD data centers, participated.

The Phase Diagrams for Ceramists Data Center, NBS, and an international team of contributing editors have finished work on Volume 4 of the Phase Diagrams for Ceramists series. It will be published shortly by the American Ceramic Society. This volume, the first published since 1975, contains 590 new diagrams with commentaries and covers metal-oxygen and metal-oxide systems and systems with oxygen-containing radicals. It is expected that Volume 5 of the series, which contains molten salts, sulfides, oxynitride systems, and aqueous systems, also will be published later this year. □

Articles Appearing in Journal of Physical and Chemical Reference Data

Bound reprints of each paper are available at the indicated price from Business Operations, Books and Journals Division, American Chemical Society, 1155 Sixteenth Street, N.W., Washington, DC 20036. Single issue copies of the **Journal** are available for $40. Checks payable to the American Chemical Society must accompany the order.



Ion Product of Water Substance, 0-1000°C, 1-10,000 Bars. New International Formulation and Its Background, W. L. Marshall and E. U. Franck, Vol. 10, No. 2, pp. 295-304, $4. Reprint #181.

Atomic Transition Probabilities for Iron, Cobalt, and Nickel: A Critical Data Compilation of Allowed Lines, J. R. Fuhr, G. A. Martin, W. L. Wiese, and S. M. Younger, pp. 305-566, $12. Reprint #182. □

New Publications

Wavelengths and Transition Probabilities for Atoms and Atomic Ions, Part I - Wavelengths, J. Reader and C. H. Corliss, **Part II - Transition Probabilities,** W. L. Wiese and G. A. Martin, NSRDS-NBS 68, 415 pp., 1980, Government Printing Office*, SN 003-003-02288-8, $14.

Optical Spectra of Nonmetallic Inorganic Transient Species in Aqueous Solution, G. L. Hug, NSRDS-NBS 69, 167 pp., 1981, Government Printing Office*, SN 003-003-02322-1, $5.50.

Data Index for Energy Transfer Collisions of Atoms and Molecules - 1970-1979, J. W. Gallagher, J. V. Blerkom, E. C. Beaty, and J. R. Rumble, NBS SP 593, 346 pp., 1981, Government Printing Office*, SN 003-003-02315-9, $8.

NBS*AIDS80: A FORTRAN Program for Crystallographic Data Evaluation, A. D. Mighell, C. R. Hubbard, and J. K. Stalick, NBS TN 1141, 54 pp., 1981, Government Printing Office*, SN 003-003-02309-4, $3.75.

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Annual Cumulation with Keyword and Author Indexes, Volume 13, 708 pp., 1980, Radiation Chemistry Data Center, Radiation Laboratory, University of Notre Dame, Notre Dame, IN 46556, $18.

*These publications are available from the Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402. (Add 25% for other than U.S. mailing.) □